A DISCRETE ELEMENT ANALYSIS OF COLLAPSE MECHANISMS IN GRANULAR MATERIALS

François NICOT
CEMAGREF, Grenoble (France)

Nejib HADDA
CEMAGREF, Grenoble (France)

Franck BOURRIER
CEMAGREF, Grenoble (France)

Luc SIBILLE
Institut de Recherche en Génie Civil et Mécanique, Université de Nantes, ECN-CNRS, Nantes (France)

Félix DARVE
UJF-INPG-CNRS, Laboratoire Sols Solides Structures Risques, Grenoble (France)

ABSTRACT: *This paper attempts to numerically examine the concept of diffuse failure using a numerical approach based on a discrete element method. First, the theoretical background is reviewed, and it is shown how the kinetic energy of a system, initially at rest after a loading history, is likely to increase under the effect of disturbances. The vanishing of the second-order work thus constitutes a basic ingredient, related to both the pioneering work of Hill (1958) and the notion of bifurcation applied to geomechanics (Vardoulakis and Sulem, 1995).*
Discrete numerical simulations were performed on homogeneous three-dimensional specimens, and the three basic conditions that must be satisfied in order to observe a failure mechanism are numerically checked: (i) the equilibrium state belongs to the bifurcation domain, in which the symmetric part of the tangent constitutive operator admits at least one negative eigenvalue; (ii) the loading is controlled by mixed parameters, some being composed of stress components, the other of strain components; and, (iii) the mixed control parameters, when maintained constant, impose a loading direction associated with a negative value of the second-order work.

KEYWORDS:
Bifurcation, sustainability, second-order work, loading parameters, discrete element method, diffuse failure, collapse.

1. INTRODUCTION

Failure in geomechanics can be analysed as a bifurcation phenomenon with loss of uniqueness and loss of stability (it should be noted that bifurcation does not necessarily imply either loss of uniqueness or loss of stability) and this seems to be true for any kind of failure mode by divergence (Darve and Vardoulakis, 2004).

To analyse failure in non-associate materials, one criterion plays a particular role: this is the so-called second-order work criterion (Bazant and Cedolin, 2003; Vardoulakis and Sulem, 1995; Darve and Vardoulakis, 2004) because – if we except flutter instabilities – this is the first to be met along a given loading path and it contains all the other classical criteria such as plastic limit conditions and strain localisation criteria (Challamel *et al*., 2009; Challamel *et al*., 2010; Nicot *et al*., 2010). However, this second-order work criterion has to be used very carefully to avoid presumable counter-examples. Clarifying the conditions for utilising this criterion properly is the main objective of this paper.

So, more precisely, three necessary and sufficient conditions have to be fulfilled for true material failure:

the stress state has to be inside the bifurcation domain;

the loading direction has to be inside an instability cone;

proper loading variables have to be chosen.

If one of these three conditions is not fulfilled, failure will not occur even if the second-order work takes strictly negative values. The second-order work criterion is no more than a necessary condition for failure. On the other hand and by excepting flutter instabilities, a strictly positive second-order work in all loading directions (i.e. for all disturbances) is a sufficient condition of stability (Hill, 1958), excluding any kind of material failure. The purpose of this paper is therefore to investigate these three necessary and sufficient conditions for failure.

This requires a numerical method able to describe a failure mechanism in detail. Today it seems that only molecular dynamics methods give reliable and robust results for the development of a failure mechanism, including pre- and post-failure regimes (by minimizing assumptions). Thus a discrete element method (Cundall and Strack, 1979) has been used.

In the first part of this paper, the notion of loss of sustainability and its correlation with the second-order work criterion is reviewed, then discrete element results are presented and discussed to check the validity of these three necessary and sufficient conditions for material failure.

2. LOSS OF SUSTAINABILITY:

Let us consider a granular sample, assumed to be a representative volume element at an equilibrium state $(\overline{\overline{\sigma}},\overline{\overline{\varepsilon}})$ under some prescribed boundary conditions. The notion of “control parameters” can be introduced: the loading applied to the sample is controlled by parameters acting on its boundaries.

Whether this state $(\overline{\overline{\sigma}},\overline{\overline{\varepsilon}})$ is sustainable if the control parameters are kept unchanged was a basic query introduced by Nicot (Nicot *et al*., 2007; Nicot and Darve, 2007).

If a new mechanical state can be reached, without changing the control parameters, then the equilibrium state is reputed to be unsustainable. As the transition from an equilibrium state toward another mechanical state is accompanied by significant increase in the kinetic energy, the loss of sustainability is related to failure. In such a case, the initial equilibrium state corresponds to a bifurcation point, since the response of the material is discontinuous under continuous evolution of control parameters (stationary).

Since the development of kinetic energy is the key point of this approach, the loss of sustainability can be related to the second-order work criterion. Starting from the balance equations written at the equilibrium state, then applying time differentiation of these equations yields a condition for kinetic energy raise from zero to a strictly positive value. By assuming small deformations and neglecting the changes in the geometrical configuration, this increase in kinetic energy coincides with zero or negative values of the second-order work W_2: $W_2 = \delta\overline{\overline{\sigma}} : \delta\overline{\overline{\varepsilon}} \leq 0$.

This approach is checked using a discrete numerical model in the following section. Thereafter, both strain or stress tensors, say $\overline{\overline{X}}$, will be replaced by a six-dimension vector $\vec{X}$.

3. THE DISCRETE ELEMENT MODEL

3.1 Numerical specimen

The numerical analyses were carried out with the 3D open source software YADE (Kozicki and Donzé, 2008) based on a discrete element method as proposed by Cundall and Strack (1979) to describe the mechanical behaviour of granular soils.

The intergranular interaction law is described by a relation of proportionality between the contact force and the relative displacement of the two spheres involved in the contact. The interaction law used in this paper includes three constant mechanical parameters k_n, k_t and φ_g. k_n is the elastic stiffness contact in the normal direction to the tangent contact plane (no tensile normal force is allowed). In the direction included in the tangent contact plane, the elastic stiffness contact is denoted by k_t. In addition, the tangential contact force obeys the Coulomb friction law characterised by a friction angle φ_g.

The discrete element model consists of a cubical sample made up of 10,000 spherical particles whose size distribution is continuous and which diameter D_s ranges from 2 to 12 mm.

The loading path (strain, stress or mixed control parameters) is imposed on the spheres assembly by controlling the positions of six rigid and purely frictionless walls in contact with spheres at the boundaries of the specimen, either directly for a strain control or indirectly through a closed-loop control for a stress control. Strain and stress responses are numerically computed at the boundary of the specimen (as in real test). In this paper, simulations are limited to axisymmetric stress-strain states ($\sigma_2 = \sigma_3$ and $\varepsilon_2 = \varepsilon_3$).

Numerical computations were performed by considering a loose specimen with an initial porosity equal to 0.42. The normal stiffness k_n at the contact between two particles is equal to 356 D_s (MN/m), the tangent stiffness k_t at the contact between particles is equal to 0.42 k_n. The friction angle φ is fixed at 35 deg.

The granular assembly was first subjected to an isotropic compression, at different confining pressure σ_3 (50, 100 and 150 kPa). Then, after each confining stage, a drained triaxial loading in axisymmetric conditions was simulated. The evolution of both $\eta = \frac{q}{p}$ (Where q denotes the deviatoric stress ($q = \sigma_1 - \sigma_3$) and p denotes the mean pressure ($p = \frac{\sigma_1 + 2\sigma_3}{3}$)) and the volumetric strain ε_v in terms of the axial strain ε_1 are given in Figs. 1 and 2 respectively.

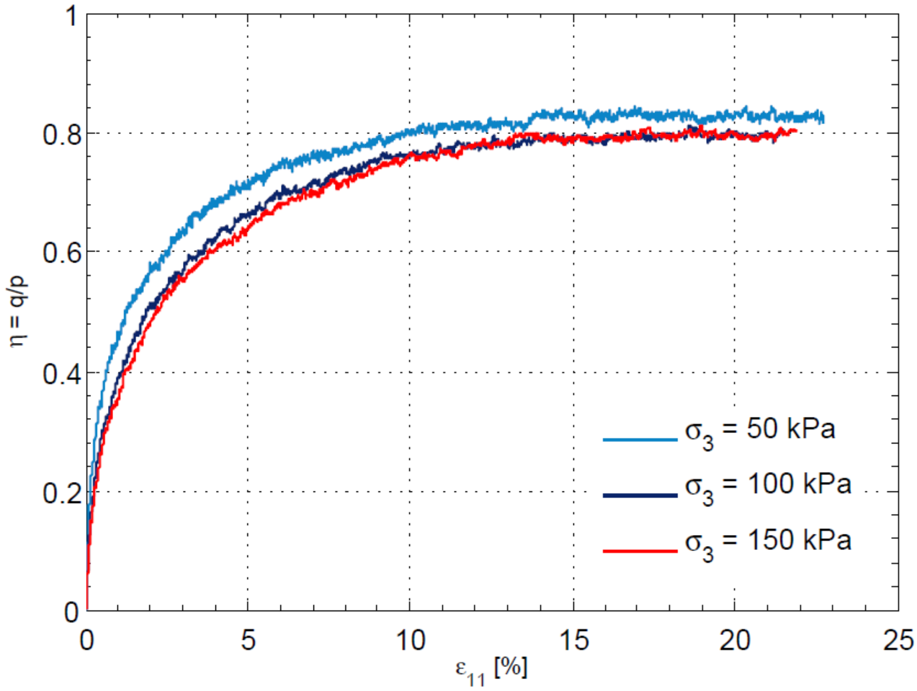

Fig. 1: Deviatoric stress ratio over the axial strain at different confining pressures

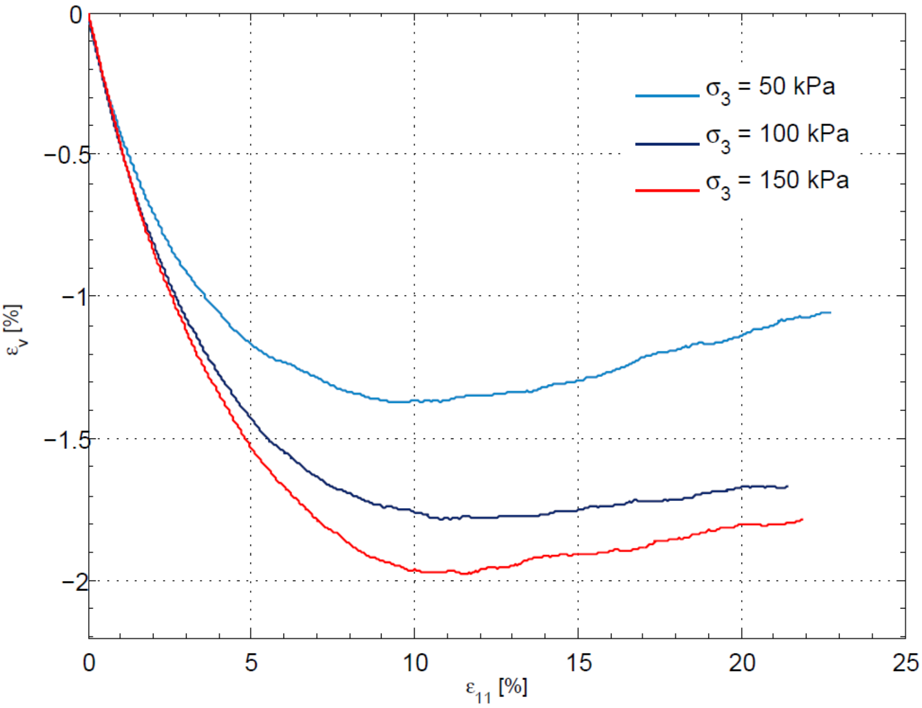

Fig. 2: Volumetric strain over the axial strain at different confining pressures

3.2 Existence of a bifurcation domain

Axisymmetric strain probes were conducted in order to compute the macroscopic second order work. Stain probes are performed from an initial stress-strain state by imposing a loading vector $\delta\vec{\varepsilon}$ defined in the Rendulic plane of strain increments ($\delta\varepsilon_1$, $\sqrt{2}\delta\varepsilon_3$) by its norm $\|\delta\vec{\varepsilon}\| = 0.0001$ and its angle α_ε between the $\sqrt{2}\delta\varepsilon_3$ axis and $\delta\vec{\varepsilon}$ (see Fig. 3a). α_ε varies from 0° to 360° by a 10° interval to check each strain direction. The corresponding response vectors $\delta\vec{\sigma}$ are simulated with the discrete element method and defined in the Rendulic plane of stress increments ($\delta\sigma_1$, $\sqrt{2}\delta\sigma_3$) (see Fig. 3b). The initial stress-strain state of strain probes results from an isotropic compression up to 100 kPa followed by an axisymmetric triaxial compression ($\sigma_2 = \sigma_3 = 100$ kPa) stopped at three stress ratios $\eta = 0.317$, $\eta = 0.553$ and $\eta = 0.628$ respectively.

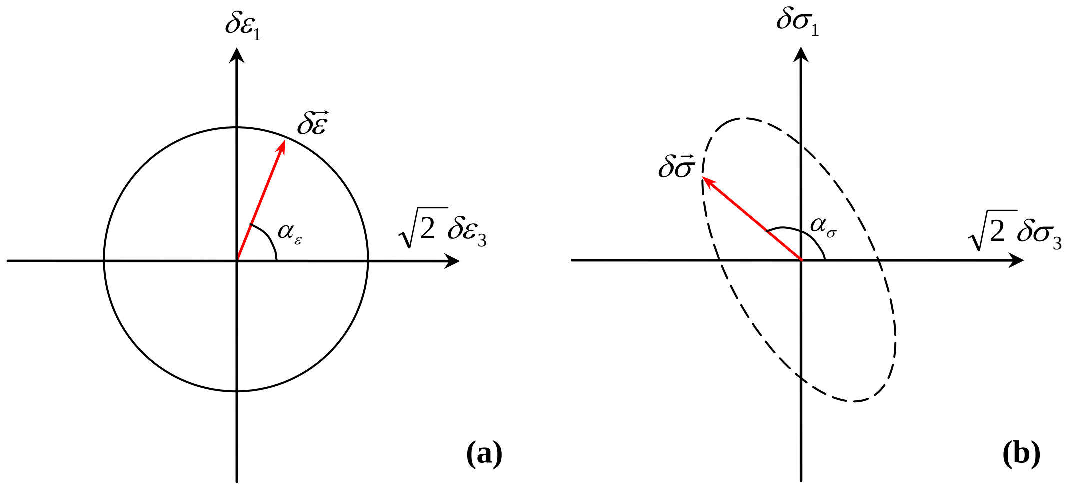

Fig. 3: Definition of strain probes (a) and stress response (b) in the axisymmetric plane of strain increments and stress increments respectively

The values of the normalized second order work: $W_2{}^n = \dfrac{\delta\vec{\sigma}\ .\ \delta\vec{\varepsilon}}{\|\delta\vec{\sigma}\|\ \|\delta\vec{\varepsilon}\|}$ corresponding to each strain probe direction can be computed once the stress increment $\delta\vec{\sigma}$ is determined for each direction of strain increment $\delta\vec{\varepsilon}$. Fig. 4 presents circular diagrams (Laoufa and Darve, 2002) of the normalized second order work $W_2{}^n$ computed from simulations of strain probes. On this diagram, each point corresponds to the extremity of a radial vector; its direction is given by angle α_ε (strain representation). For convenience, an arbitrary constant $c = 0.5$ is added to the polar value of $W_2{}^n$. A dashed circle is drawn in the circular diagram to represent vanishing values of $W_2{}^n$. $W_2{}^n$ is positive outside the dashed circle, and is negative inside.

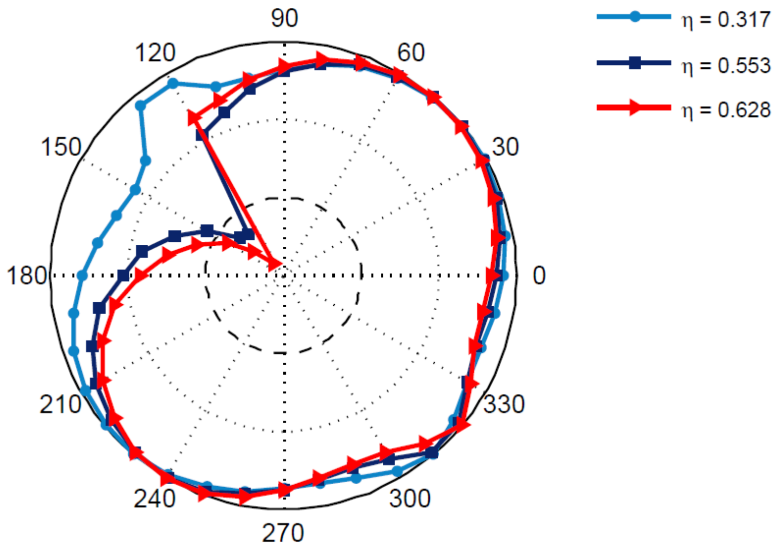

Fig. 4: Circular diagrams of the second-order work at a confining pressure of 100 kPa

It can be seen that the second order work takes negative values along the strain direction included within a cone, for a deviatoric stress ratio larger than approximately 0.5. The opening angle of the cone increases with the deviatoric stress ratio as the stress state gets closer to the Mohr-Coulomb failure line. The existence of cones of unstable strain directions shows that the discrete numerical sample possesses a wide bifurcation domain. Its boundary is clearly within the plastic limit surface which means that various types of failure can occur before reaching the plastic limit.

4. SIMULATIONS OF THE LOSS OF SUSTAINABILITY

It has been shown via the directional analysis in the previous section that negative values of the second-order work do exist for the numerical specimen at a deviatoric stress ratio $\eta = 0.628$; the corresponding mechanical state belongs therefore to the bifurcation domain. The unstable cone is limited by two directions corresponding to $\alpha_\varepsilon = 120°$ and $\alpha_\varepsilon = 155°$ in the Rendulic plane of strain increments ($\delta\varepsilon_1$, $\sqrt{2}\delta\varepsilon_3$). These two limiting angles can be expressed in the Rendulic plane of stress increments ($\delta\sigma_1$, $\sqrt{2}\delta\sigma_3$) using the following relation and taking into account the signs of stress responses: $\alpha_\sigma = \arctan\left(\frac{\delta\sigma_1}{\sqrt{2}\delta\sigma_3}\right)$, which returns $\alpha_\sigma = 215°$ and $\alpha_\sigma = 235°$ respectively as limit angles of the cone of unstable directions in the Rendulic plane of stress increments.

Setting $R_\sigma = \frac{1}{\sqrt{2}\tan\alpha_\sigma}$, it follows that in axisymmetric conditions stress response directions are defined by: $\delta\sigma_1 - \frac{1}{R_\sigma}\delta\sigma_3 = 0$.

As the second-order work can be expressed as follows:

$$W_2 = \delta\varepsilon_1(\delta\sigma_1 - \frac{1}{R_\sigma}\delta\sigma_3) + (\delta\varepsilon_1 + 2R_\sigma\delta\varepsilon_3)\frac{\delta\sigma_3}{R_\sigma} \qquad (1)$$

it is relevant to choose the following control parameters: $C_1 = (\delta\sigma_1 - \frac{1}{R_\sigma}\delta\sigma_3)$ and $C_2 = (\delta\varepsilon_1 + 2R_\sigma\delta\varepsilon_3)$. Then, the sustainability of the equilibrium state controlled through parameters C_1 and C_2 is checked for R_σ values corresponding to stress directions inside or outside the cone of unstable directions.

The sample, initially in an equilibrium state (at which the kinetic energy is equal to 7 10^{-6} J), is perturbed by imposing an instantaneous velocity in a random direction on eight grains belonging to the weak contact network that were chosen randomly (Sibille *et al*, 2009). The perturbation corresponds to an external input of kinetic energy of 2.10^{-5} J (the maximal value of energy developed by the numerical sample during a strain probe from the initial state is about 10^{-3} J). The responses of the numerical specimen after the perturbation of the initial state under a confining pressure of 100 kPa and controlled by both control parameters C_1 and C_2 (maintained constant) using different values of R_σ (namely α_σ) are shown in Fig. 5. The arrow indicates the time when the perturbation was applied. The response of the specimen for a stress direction characterized by $R_\sigma = 0.843$ ($\alpha_\sigma = 220°$) chosen inside the unstable cone corresponds to a sudden increase in the kinetic energy, that is, to the loss of sustainability (Nicot *et al*., 2007). The kinetic energy increases in an exponential way, and takes values after 0.035 second thousands times greater than that provided to the specimen when applying the perturbation. The equilibrium of the specimen cannot be sustained. The external stress loading cannot be balanced anymore by the internal stress whose components decrease. The specimen merely collapses.

On the contrary, for the stress directions bordering on the cone, characterized by $R_\sigma = 0.593$ and $R_\sigma = 4.01$ ($\alpha_\sigma = 230°$ and $190°$ respectively), and directions outside the cone characterized by $R_\sigma = 1.94$ and $R_\sigma = 0.286$ ($\alpha_\sigma = 200°$ and $254°$ respectively), the kinetic energy vanishes after some initial bursts. The mechanical state of the specimen remains more or less unchanged and both external stress and strain components stabilize at values very near to the initial one (not shown here). No loss of sustainability and no bifurcation are observed.

Similar results were obtained by Sibille as well, using a different computational software based on a discrete element method (Sibille *et al*, 2008 and 2009; Nicot *et al*, 2009). They revealed that, well before the standard Mohr-Coulomb limit is reached and for the unstable stress directions detected by the vanishing of the second-order work, some control parameters can be chosen to lead the granular material to failure.

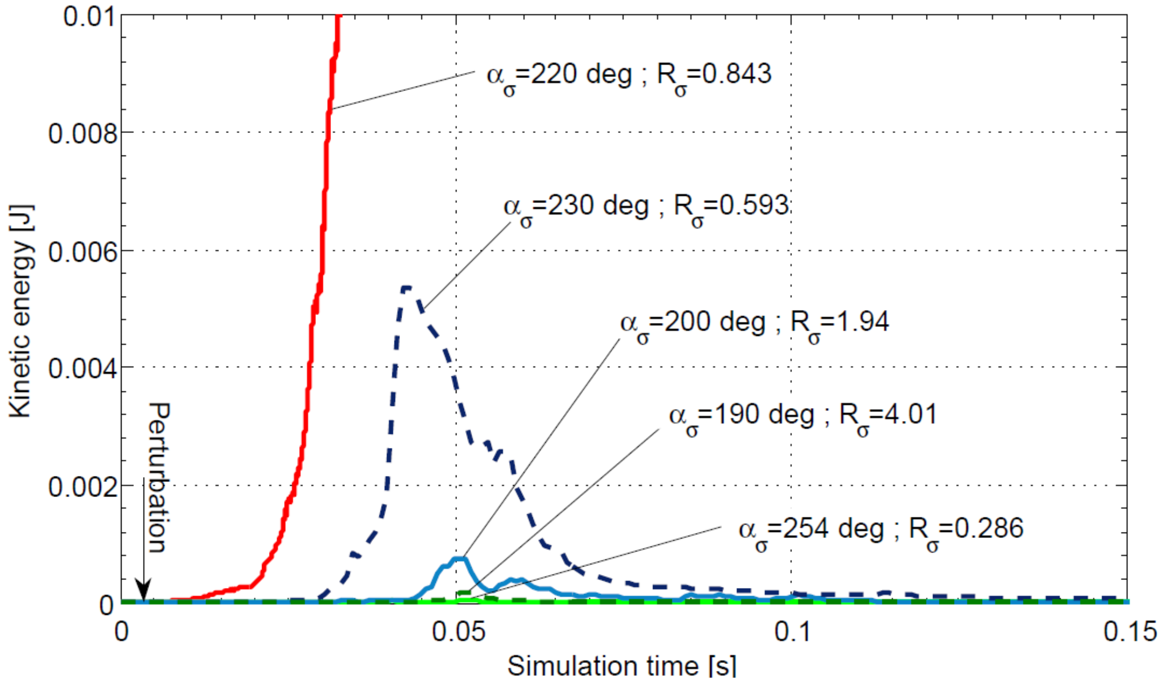

Fig. 5: Kinetic energy of the specimen after a perturbation is applied in different stress directions

5. CONCLUDING REMARKS

This paper has presented the notion of failure, described as the occurrence of an increase in kinetic energy under constant loading parameters. This notion based on theoretical findings was ascertained from three-dimensional numerical simulations based on a discrete element method. In particular, it was thoroughly verified that three basic conditions must be fulfilled to give rise to a failure mechanism:

The equilibrium state belongs to the bifurcation domain. In this domain, loading directions exist along which the second-order work takes negative values.

The loading is controlled by mixed parameters, some being composed of stress components, the other of strain components.

The mixed control parameters, when maintained constant, impose a loading direction associated with a negative value of the second-order work.

REFERENCES

Bazant Z., Cedolin L. (2003): Stability of Structures, Dover Edition Publ.

Challamel, N., Nicot, F., Lerbet, J., and Darve, F. (2009): On the stability of non-conservative elastic systems under mixed perturbations. Eur. J. Env. and Civil Eng., Vol. 13(3), pp. 347-367.

Challamel, N., Nicot, F., Lerbet, J., Darve, F. (2010): Stability of non-conservative elastic structures under additional kinematics constraints. Eng. Struct., in press.

Cundall, P.A., and Strack, O.D.L. (1979): A discrete numerical model for granular assemblies. Geotechnique, Vol. 29 (1), pp. 47-65.

Darve, F., and Vardoulakis, I. (2004): Degradations and Instabilities in Geomaterials. Springer Wien New York Publ.

Darve, F., Servant, G., Laouafa, F., and Khoa H.D.V. (2004): Failure in geomaterials, continuous and discrete analyses. Comp. Methods Appl. Mech. Engrg., Vol. 193, pp. 3057-3085.
Hill, R. (1958): A general theory of uniqueness and stability in elastic-plastic solids. J. Mech. Phys. Solids, Vol. 6, pp. 236-249.
Kozicki, J., and Donzé, F.V. (2008): A new open-source software developed for numerical simulations using discrete modeling methods. Comp. Meth. Appl. Mech. and Eng., Vol. 197(49-50), pp. 4429-4443.
Laouafa, F., and Darve, F. (2002): Modelling of slope failure by a material instability mechanism. Comp. and Geotech., Vol. 29(4), pp. 301-325.
Nicot, F., and Darve, F. (2007): A micro-mechanical investigation of bifurcation in granular materials. Int. J. of Solids and Structures, Vol. 44, pp. 6630-6652.
Nicot, F., Challamel, N., Lerbet, J., and Darve, F. (2010): Mixed loading conditions, revisiting the question of stability in geomechanics. Int. J. of Num Anal Methods in Geomechanics, Article first published online: 2 SEP 2010 | DOI: 10.1002/nag.959.
Nicot, F., Darve, F., and Khoa, H.D.V. (2007): Bifurcation and second-order work in geomaterials. Int. J. Num. Anal. Methods in Geomechanics, Vol. 31, pp. 1007-1032.
Nicot, F., Sibille, L., and Darve, F. (2009): Bifurcation in granular materials: an attempt at a unified framework. Int. J. of Solids and Structures, Vol. 46, pp. 3938–3947.
Sibille, L., Donzé, F., Nicot, F., Chareyre, B., and Darve, F. (2008): Bifurcation detection and catastrophic failure. Acta Geotecnica, Vol. 3(1), pp. 14-24.
Sibille, L., Nicot, F., Donzé, F., and Darve, F. (2009): Analysis of failure occurrence from direct simulations. European J. Environmental and Civil Eng., Vol. 13(2), pp. 187-202.
Vardoulakis, I., and Sulem, J. (1995): Bifurcation analysis in geomechanics. Chapman & Hall Publisher, London.